ROTATIONAL SPECTROSCOPY OF MONOFLUOROETHANOL AGGREGATES WITH ITSELF AND WITH WATER

JAVIX THOMAS, WENYUAN HUANG, XUNCHEN LIU[a], WOLFGANG JÄGER, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*.

Fluoroalcohols are used as common cosolvents for studies of the secondary and tertiary substructures of polypeptides and proteins in aqueous solution. It has been proposed that small fluoroalcohol aggregates are crucial for the protein structural altering process.[1] A rotational spectroscopic study of the monofluoroethanol (MFE) dimer was reported by our group before.[2] In this presentation, we report our recent results on the MFE trimer and MFE-water clusters. We analyze the competitive formation of intra- and intermolecular hydrogen bonds, processes that may be crucial for the changes in protein structure that occur in fluoroalcohol-water solution. We show that the MFE trimer takes on a much different binding topology from the recently reported phenol trimer.[3] The results will also be compared to the closely related 2,2,2-trifluoroethanol systems.

[1] H. Reiersen, A. R. Rees, Protein Eng. 2000, 13, 739 – 743. [2] X. Liu, N. Borho, Y. Xu, Chem. Eur. J. 2009, 15, 270 – 277. [3] a) N. A. Seifert, A. L. Steber, J. L. Neill, C. Pérez, D. P. Zaleski, B. H. Pate, A. Lesarri, Phys. Chem. Chem. Phys., 2013, 15, 11468; b) T. Ebata, T. Watanabe, N. Mikami, J. Phys. Chem., 1995, 99, 5761.

[a]Permanent address: Mechanical Department, Shanghai Jiao Tong University, Shanghai, P. R. China.